

Phonon mediated correlation effects on the transport properties of a benzene molecular transistor

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We analyze theoretically correlation effects on the transport properties of a benzene molecular transistor, that are mediated by interactions between the motion of the nuclei and the transmitted charge. We focus on a single phononic mode which allows us to derive an analytic expression for the current. The results provide transparent interpretations of various features of the highly nonlinear current-voltage characteristics, which is experimentally accessible through resonant inelastic electron tunneling spectroscopy. The theoretical approach we present is generally applicable to correlated nano-scale devices and considers exactly electron-electron interactions and the coupling to vibrational degrees of freedom in the device while the tunneling coupling to the leads is treated perturbatively.

Vibrations of atoms in molecules or solids play an important role for many intriguing phenomena in various fields of physics. In condensed matter physics novel states often emerge from phonon mediated collective behavior. Among them are conventional superconductivity [1], colossal magnetoresistance [2], and thermoelectricity [3]. Localized vibrational modes are also believed to stabilize the α -helix in protein and to be responsible for storage and transport processes [4]. In molecular electronics, the electron-phonon interactions strongly influence the conduction properties, contribute significantly to heating, and lead to nonlinear effects, including bistability, negative differential conductance, and hysteretic behavior [5–16]. In these systems signatures of the interaction between charge carriers and molecular vibrations can be faithfully characterized by (resonant) inelastic electron tunneling [(R)IET] spectroscopy [15, 17, 18]. The importance of phonon modes on the conduction properties of molecular transistors has been demonstrated in various seminal experiments [19–26].

A wide range of theoretical studies concerning nonequilibrium properties of nanoscale devices are based on the nonequilibrium Green's function (NEGF) method evaluated in the frame of the local density approximation (LDA) (see e.g. [27, 28] and references therein). On the one hand, the LDA-NEGF approach is *ab-initio* and as such allows to study realistic devices, on the other hand, correlation effects, irrespective whether they are of electron-electron or electron-phonon character, are included only to low order. This can lead to unphysical results provided the interaction is strong [29].

In the theoretical approach, presented here, we start out from the exact expression for the current within the NEGF framework and employ a strong coupling cluster approximation to evaluate the required Green's functions (GF) [30, 31]. This allows to exactly take into account all interaction of the nanoscale device itself, be it of electron-electron or electron-phonon nature, while treating the influence of the leads perturbatively. As an

application, we investigate the nonequilibrium transport across a *benzene* molecular transistor [Fig. 1 (a)] and observe that at low temperatures phonon mediated interactions leave a phononic fingerprint qualitatively similar to those observed in (R)IET spectroscopy [19–26].

At low temperatures we obtain a stepwise increase of the current at voltage differences given by twice the phonon energy, Fig. 1 (b). The stepwise increase of the current manifests in the conductance and in the differential shot noise through multiple, equally-spaced peaks, Fig. 1 (c) and (d), as well as in a branching of the diamond structure in the stability diagram, Fig. 3. At low bias voltage the current is significantly suppressed due to electron-phonon interactions, which is reminiscent of the Franck-Condon blockade in molecular devices [6], see inset of Fig. 1 (b).

Theoretical description.—We consider a molecular transistor consisting of a single benzene aromatic ring coupled to metallic leads, Fig. 1 (a). The benzene molecule is modeled by the Hamiltonian

$$H_b = H_e + H_p + H_{ep} . \quad (1)$$

The first term describes the motion of the electrons,

$$H_e = \sum_{i,\sigma} \left[-t(c_{i\sigma}^\dagger c_{i+1\sigma} + \text{h.c.}) + \epsilon c_{i\sigma}^\dagger c_{i\sigma} \right] ,$$

where t is the hopping amplitude and ϵ the local energy, which can be controlled by the gate voltage V_g , i.e., $\epsilon \rightarrow \epsilon + eV_g$. Electrons with spin σ on orbital i are created (destroyed) by $c_{i\sigma}^\dagger$ ($c_{i\sigma}$). The second term H_p is the bare phonon part, which we transform into the eigenmodes

$$H_p = \sum_m \hbar\omega_m b_m^\dagger b_m ,$$

where b_m^\dagger (b_m) create (destroy) phonons in mode m with energy $\hbar\omega_m$. The last term in (1) incorporates the Su-Schrieffer-Heeger [32] electron-phonon interaction

$$H_{ep} = \sum_{mj\sigma} g_m D_m^{(j,j+1)} (b_m^\dagger + b_m) (c_{j\sigma}^\dagger c_{j+1\sigma} + \text{h.c.})$$

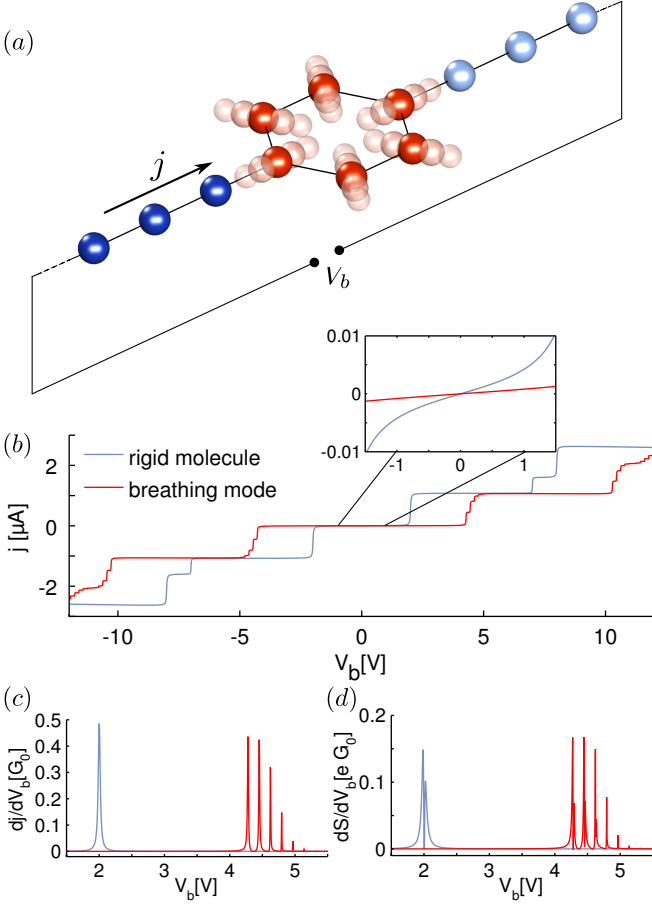


FIG. 1. (Color online) (a) Illustration of the phonon breathing mode in a benzene molecular transistor (red spheres) which is coupled to metallic leads (blue spheres). (b) The bias voltage V_b induces a current j that is significantly modified by the interaction between the nuclear motion and the charge. At low V_b the current is suppressed [6], see inset, whereas at large V_b strong nonlinear behavior leads to a stepwise increase of the current, also manifesting in (c) the conductance and (d) the differential shot noise through multiple equally spaced peaks. The data is evaluated at $T = 10\text{K}$.

with $g_m := g\sqrt{\hbar/2M\omega_m}$, g the electron-phonon interaction, M the mass of the nuclei, and D_m the displacement matrix of eigenmode m , which is given by

$$D_m^{(j,j+1)} = \frac{1}{\sqrt{6}} e^{i\frac{\pi}{3}mj} \quad \text{with } m \in \{0, 1, \dots, 5\}.$$

The metallic leads are described by semi-infinite tight-binding chains with hopping t_α , on-site energy ϵ_α , and chemical potential μ_α ($\alpha = \text{left or right}$). We assume that the bias voltage $eV_b = \mu_l - \mu_r$ is applied symmetrically, i.e., $\mu_l = \epsilon_l = -\mu_r = -\epsilon_r$ and that the leads are equilibrated, i.e., that the occupation follows the Fermi-Dirac statistics $f_\alpha = [e^{(\epsilon - \mu_\alpha)/k_B T} + 1]^{-1}$, where k_B is the Boltzmann constant and T the temperature.

In this work we use the NEGF framework to evalu-

ate the nonequilibrium steady-state properties along the lines presented in [30]. Due to the electron-phonon interaction it is in general not possible to solve the problem exactly and thus we employ Cluster Perturbation Theory (CPT) [33]: In short, the system is first divided into several clusters, each of which can be solved exactly either analytically or numerically, taking correlations on the cluster level into account exactly. Strong coupling CPT is then employed to connect the individual clusters.

Here, we divide the molecular transistor into three clusters: (i) the central region consisting of the benzene ring with vibrational degrees of freedom and (ii) the left and (iii) right metallic leads which are connected to the molecular device. From the exact solution of the isolated interacting central region we obtain an approximate self-energy of the full system. The results can also be systematically improved by incorporating lead sites into the central system [30, 31]. Based on considerations similar to those of Meir and Wingreen [34] we have shown [35] that within this CPT approach the current is of the Landauer-Büttiker form [36, 37] even though correlations are included exactly on the cluster level. In particular, we find

$$j = \frac{e}{\hbar} \int \frac{d\varepsilon}{2\pi} (f_l - f_r) \text{Tr}[\mathcal{T}], \quad (2)$$

where \mathcal{T} is the transmission coefficient matrix

$$\mathcal{T} := \mathcal{G}^R(\varepsilon) \Gamma_r(\varepsilon) \mathcal{G}^A(\varepsilon) \Gamma_l(\varepsilon). \quad (3)$$

This matrix contains the retarded (advanced) GF \mathcal{G}^R ($\mathcal{G}^A = (\mathcal{G}^R)^\dagger$) which within CPT is given by $(\mathcal{G}^R)^{-1} = (g^R)^{-1} - (\tilde{\Sigma}_l + \tilde{\Sigma}_r)$, where g^R is the exact retarded GF of the isolated benzene molecule, $\tilde{\Sigma}_\alpha := T_{c\alpha} g_{\alpha\alpha}^R T_{\alpha c}$ takes into account the effect of lead α on the GF, $T_{c\alpha}$ is the tunneling coupling between the central device and lead α , and $g_{\alpha\alpha}^R$ stands for the retarded lead GF [30]. In addition, the transmission \mathcal{T} depends on the imaginary part of the lead induced self-energy via $\Gamma_\alpha = -2\text{Im} \tilde{\Sigma}_\alpha$. Similarly, the expression for the shot noise, i.e., current-current correlations, in the zero frequency limit reads [38]

$$S(\omega \rightarrow 0) := S = \frac{e^2}{\hbar} \int \frac{d\varepsilon}{2\pi} [f_l(1 - f_l) + f_r(1 - f_r)] \text{Tr}[\mathcal{T}] + (f_l - f_r)^2 \text{Tr}[(1 - \mathcal{T})\mathcal{T}]. \quad (4)$$

In principle the nonequilibrium properties can be determined by solving the eigenvalue problem of H_b numerically taking all phonon modes into account using the formulas discussed above. Within this approach it is also straight forward to introduce electron-electron interactions giving rise to Kondo physics provided the molecule is (asymmetrically) electron or hole doped [39].

In the present work, however, we want to focus on the effects generated by the electron-phonon interaction. In order to gain insight into the problem we focus on a single phonon mode, in particular on the breathing mode

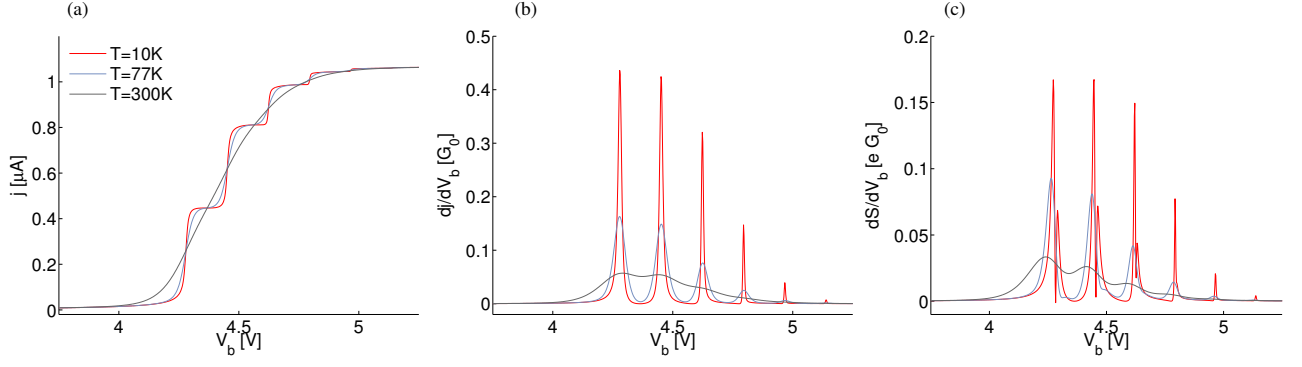


FIG. 2. (Color online) Temperature dependence of (a) the current, (b) the conductance, and (c) the differential shot noise versus bias voltage V_b curves. At temperatures T much lower than the phonon energy $\omega_\mu = 0.086\text{eV}$, which is the smallest energy scale in Eq. (1), the phonon mediated steps and peaks, respectively, are pronounced and clearly visible. For increasing temperature these features are washed out and at room temperature $T = 300\text{K}$ hardly any remain.

illustrated in Fig. 1(a), which is the one with the lowest excitation energy ω_μ of the isolated benzene ring. Another appealing feature of this mode is the fact that the resulting interacting model of the central region can be solved analytically and allows to obtain a transparent insight into the non-equilibrium physics of such a molecular electronic device.

Analytic solution.—For a single phonon mode μ (not necessarily the breathing mode) we can readily eliminate the electron-phonon interaction by a unitary transformation of the Lang-Firsov type [28]. To this end we first diagonalize the displacement matrix $D_\mu X = X\Lambda$, Λ is the diagonal matrix with the eigenvalues and X the corresponding matrix of eigenvectors, and transform the electron operators accordingly $\mathbf{d} = X\mathbf{c}$, where we introduce the vector notation $\mathbf{c}^\dagger = (c_{1\uparrow}^\dagger, c_{2\uparrow}^\dagger, \dots, c_{L\downarrow}^\dagger)$. The Lang-Firsov like unitary transformation is generated by the operator

$$e^S := e^{\frac{g_\mu}{\hbar\omega_\mu}(b-b^\dagger)\mathbf{d}^\dagger\Lambda\mathbf{d}}. \quad (5)$$

All operators that are subject to the unitary transformation are denoted by $\bar{O} := e^S O e^{-S}$, which in particular results in

$$\bar{d}_{k\sigma}^\dagger = d_{k\sigma}^\dagger e^{\frac{g_\mu}{\hbar\omega_\mu}(b-b^\dagger)\lambda_k}. \quad (6)$$

The Lang-Firsov transformation eliminates the explicit electron phonon interaction and results in an effective Hamiltonian $\bar{H}_b = \bar{H}_e + \hbar\omega_\mu b^\dagger b$. The electronic GF entering the transport properties of the molecular junction [Eq. (3)] is transformed accordingly, i.e., $g(k, \omega) \rightarrow \bar{g}(k, \omega)$ by replacing $d_{k\sigma}^\dagger \rightarrow \bar{d}_{k\sigma}^\dagger$ in its definition. For the particular case of the breathing mode the matrices D_μ and the matrix describing the nearest neighbor hopping commute and thus can be diagonalized by a common set of eigenvectors. In this case we find $\lambda_k = \sqrt{2/3} \cos k$ and $X_{nk} = \exp(ikn)/\sqrt{6}$. The $d_{k\sigma}^\dagger$ thus create electrons with

a given (angular) momentum k in the molecule. In the transformed Hamiltonian the electronic part becomes

$$\bar{H}_e = \sum_{k\sigma} (\epsilon - 2t \cos k) n_{k\sigma} - U \left(\sum_{k\sigma} n_{k\sigma} \cos k \right)^2. \quad (7)$$

After this transformation, the electron and phonon degrees of freedom are completely decoupled but instead an attractive electron-electron interaction proportional to $U := \frac{2g_\mu^2}{3\hbar\omega_\mu}$ emerges. This interacting Hamiltonian can be solved exactly. The eigenvectors are of the form $|n\rangle |K_\uparrow\rangle |K_\downarrow\rangle$, i.e., they are tensor products of the oscillator eigenvectors $|n\rangle$ and the slater determinants $|K_\sigma\rangle := \prod_{k \in K_\sigma} \bar{d}_{k\sigma}^\dagger |0\rangle$ composed of the molecular orbital operators $\bar{d}_{k\sigma}^\dagger$ dressed by bond-distortions that are encoded in the Lang-Firsov factor of Eq. (6). For the electron GF for a single spin-species we find

$$\bar{g}(k, \omega) = \sum_n \frac{e^{-\alpha_k^2} \alpha_k^{2n}}{n!} \left[\frac{\Theta(k > k_F)}{\hbar\omega - (E_{kn}^+ - E_0)} + \frac{\Theta(k < k_F)}{\hbar\omega + (E_{kn}^- - E_0)} \right] \quad (8)$$

with $\alpha_k = \sqrt{U} \cos k$ and the energies are

$$\begin{aligned} E_0 &= \epsilon \mathcal{N}_0 - 2t\mathcal{C}_0 - U\mathcal{C}_0^2 \\ E_{kn}^\pm &= n\hbar\omega_\mu + (\mathcal{C}_0 \pm 1)\epsilon - 2t(\mathcal{C}_0 \pm \cos k) - U(\mathcal{C}_0 \pm \cos k)^2 \\ \mathcal{C}_0 &= \sum_\sigma \sum_{q \in \text{FS}} \cos q. \end{aligned}$$

\mathcal{N}_0 is the equilibrium number of electrons in the benzene molecule and FS denotes the Fermi sea. The physical properties of the system are particularly obvious in the differential conductance which to order $O(V_b^2/T^2)$ and $O(t^2/t_\alpha^2)$ is given by

$$\frac{dj}{dV_b} = \frac{e}{4\hbar\pi} [\mathcal{T}(V_b/2) + \mathcal{T}(-V_b/2)]. \quad (9)$$

Along with Eqs. (3) and (8) it can be deduced that current pathways open up, whenever $V_b/2$ is equal to an the excitation energy $\hbar\omega = E_{kn}^+ + \hbar\omega_\mu n$ in the particle sector or $\hbar\omega = -E_{kn}^- + \hbar\omega_\mu n$ in the hole sector.

Transport properties.—Next, the impact of phonons on the transport properties shall be investigated guided by the breathing mode of a benzene molecular transistor. We use the parameters reported in [13, 40] for the benzene molecule and the electron phonon coupling; in particular we set $t = 2.5\text{eV}$, $\epsilon = -1.5\text{eV}$, $\hbar\omega_\mu = \sqrt{K/M} = 0.086\text{eV}$, and $g_\mu = 0.18\text{eV}$. In addition, for the metallic leads we choose $t_\alpha = 12\text{eV}$ close to the wideband limit and the coupling between the leads and the benzene ring is $t' = 0.4\text{eV}$. Therefore the smallest energy scale in the model is the phonon energy $\hbar\omega_\mu$. The current evaluated at $T = 10\text{K}$ (the temperature enters through the Fermi-Dirac distribution functions of the leads) for the rigid molecule as well as the molecule with the breathing phonon mode is shown in Fig. 1 (b). At low bias voltage we observe a suppression of the current due to electron-phonon interactions, reminiscent of the Franck-Condon blockade [6], see inset. Due to the electron-phonon mediated correlations (second term in Eq. (7)) the gap in the density of states of the benzene molecule widens considerably. Consequently, the threshold for the current increases to $V_b \sim 4\text{eV}$. Above the threshold the current increases stepwise, at voltage differences given by twice the phonon energy $\hbar\omega_\mu$, until the next plateau is reached. The new current pathways are related to the phonon excitations and the factor 2 is due to the argument $V_b/2$ in Eq. (9).

This also manifests in the differential conductance Fig. 1 (c) and in the differential shot-noise (d) through pronounced, equally spaced peaks. At the maxima of the conductance, the differential shot-noise, corresponding to the derivative of the current-current correlation for $\omega \rightarrow 0$, exhibits dips [38]. At low temperatures this is observable for a few low-energy peaks of the phonon branching. A detailed analysis of the differential conductance shows that the peaks are near the poles of the cluster GF \tilde{g} of the decoupled device. This is reasonable, since the effective coupling V/t'^2 is small. Therefore, the impact of $\tilde{\Sigma}_\alpha$ stems primarily from its imaginary part which determines the width and the weight of the individual peaks. So the measurement of these quantities can be used as a diagnostic tool to analyze the device and extract information about the electronic and the phononic excitations. In particular the equidistant peaks in the conductance and the tips in the differential shot-noise are a fingerprint of the bare phonon excitations. One should notice, however, that for general phonon modes this is not entirely correct, since the electronic excitations will depend on the phonon occupation n , due to \tilde{H}_e .

For increasing ambient temperature the phonon features are smeared out, since the phonon energy $\omega_\mu = 86\text{meV}$ is rather small and comparable to room temper-

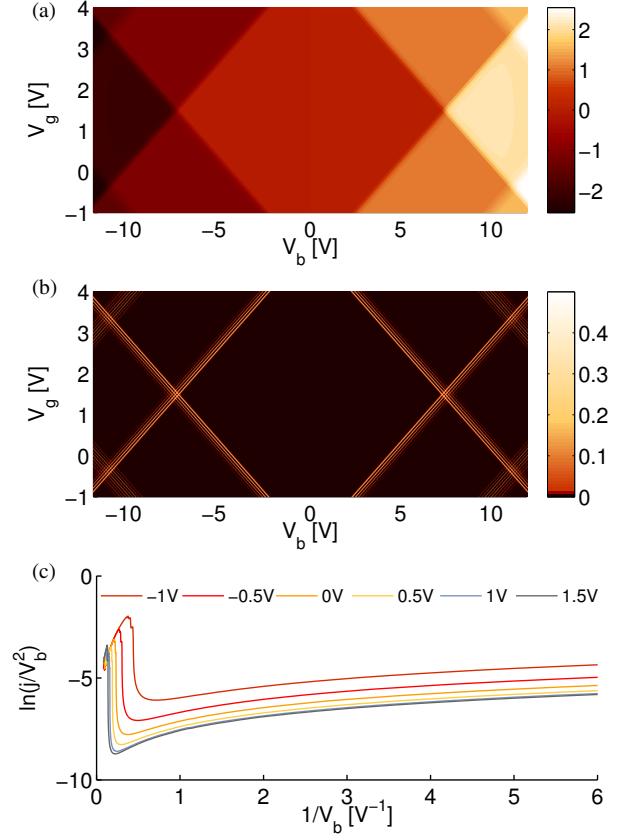


FIG. 3. (Color online) (a) Current as a function of the bias voltage V_b and the gate voltage V_g and (b) corresponding stability diagram (i.e., differential conductance). The electron-phonon interaction increases the area of the central diamond and induces a splitting of the lines in the stability diagram. (c) Fowler-Nordheim plots for a few selected values of the gate voltage V_g specified in the legend. Data evaluated for $T = 10\text{K}$.

ature $T = 300\text{K} = 26\text{meV}$. In Fig. 2, the current, the differential conductance, and the differential shot noise are shown at different temperatures $T = \{10, 77, 300\}\text{K}$. With increasing temperature the steps in the current are smoothed out and the peaks in the current and the differential shot noise decrease significantly. In addition, the dips in the shot noise vanish.

Finally, we study the consequence of orbital gating, where the local on-site energy of the benzene molecule is changed by a gate voltage, which we restrict to the HOMO-LUMO gap of the noninteracting molecule. The current as a function of the gate voltage V_g and the bias voltage V_b exhibits the celebrated diamond structure centered around particle-hole symmetric point $V_g = 1.5\text{V}$, Fig. 3 (a). As compared to the rigid molecule the area of the center diamond is increased due to the electron-phonon interactions and the transition between the diamonds involve several steps, best visible in the stability

diagram, corresponding to the conductance in the V_g - V_b plane, shown in Fig. 3(b). The Fowler-Nordheim plots (c) which show $\ln(j/V_b^2)$ as a function of V_b^{-1} compare well with the experimental observation in Ref. [26]. From these plots different tunneling regimes become apparent: At low bias voltage, the “logarithmic” dependence indicates direct tunneling, whereas for increasing bias voltage the curve has a large negative slope, indicating field emission [26]. Close to this bias voltage phonon mediated interactions manifest as small wiggles in the curves. When further increasing the voltage the next plateau is reached which is accompanied by a reentrance in the direct tunneling regime. Similarly to [26] the minimum of the curves move to larger bias voltage for increasing gate voltage reflecting the diamond shape of Fig. 3(a) and (b).

Conclusions and Outlook.— In summary, we explored phonon mediated correlation effects on the transport properties of a single benzene-ring transistor. We focused on an analytically tractable single-mode model that reveals a deeper understanding of the impact of phonons on experimental (R)IET spectra. The theoretical approach we presented allows to determine non-equilibrium properties of strongly correlated nano-scale devices. When solving the interacting device totally numerically, it also allows to include other phonon modes and electron-electron interactions.

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- [1] J. Bardeen, L. N. Cooper, and J. R. Schrieffer, *Phys. Rev.* **108**, 1175 (1957).
 - [2] A. J. Millis, *Phil. Trans. R. Soc. Lond. A* **356**, 1473 (1998).
 - [3] O. Delaire, J. Ma, K. Marty, A. F. May, M. A. McGuire, M.-H. Du, D. J. Singh, A. Podlesnyak, G. Ehlers, M. D. Lumsden, and B. C. Sales, *Nat. Mater.* **10**, 614 (2011).
 - [4] A. Scott, *Phys. Rep.* **217**, 1 (1992).
 - [5] K. Flensberg, *Phys. Rev. B* **68**, 205323 (2003).
 - [6] J. Koch and F. von Oppen, *Phys. Rev. Lett.* **94**, 206804 (2005).
 - [7] M. Galperin, A. Nitzan, and M. A. Ratner, *Phys. Rev. B* **73**, 045314 (2006).
 - [8] D. A. Ryndyk, M. Hartung, and G. Cuniberti, *Phys. Rev. B* **73**, 045420 (2006).
 - [9] C. Benesch, M. Čížek, M. Thoss, and W. Domcke, *Chem. Phys. Lett.* **430**, 355 (2006).
 - [10] D. A. Ryndyk and G. Cuniberti, *Phys. Rev. B* **76**, 155430 (2007).
 - [11] M. Galperin, M. A. Ratner, and A. Nitzan, *J. Phys.: Condens. Matter* **19**, 103201 (2007).
 - [12] M. Galperin, M. A. Ratner, A. Nitzan, and A. Troisi, *Science* **319**, 1056 (2008).
 - [13] A. L. Botelho, Y. Shin, M. Li, L. Jiang, and X. Lin, *J. Phys.: Condens. Matter* **23**, 455501 (2011).
 - [14] G. Cuniberti, K. Richter, and G. Fagas, *Introducing Molecular Electronics*, 1st ed. (Springer, Heidelberg, Germany, 2005).
 - [15] J. C. Cuevas and E. Scheer, *Molecular Electronics: An Introduction to Theory and Experiment (Nanotechnology and Nanoscience)*, 1st ed. (World Scientific Publishing Company, Singapore, 2010).
 - [16] H. Song, M. A. Reed, and T. Lee, *Advanced Materials* **23**, 15831608 (2011).
 - [17] R. C. Jaklevic and J. Lambe, *Phys. Rev. Lett.* **17**, 1139 (1966).
 - [18] B. C. Stipe, M. A. Rezaei, and W. Ho, *Science* **280**, 1732 (1998).
 - [19] H. Park, J. Park, A. K. L. Lim, E. H. Anderson, A. P. Alivisatos, and P. L. McEuen, *Nature* **407**, 57 (2000).
 - [20] N. Zhitenev, H. Meng, and Z. Bao, *Phys. Rev. Lett.* **88**, 226801 (2002).
 - [21] R. H. M. Smit, Y. Noat, C. Untiedt, N. D. Lang, M. C. v. Hemert, and J. M. v. Ruitenbeek, *Nature* **419**, 906 (2002).
 - [22] X. H. Qiu, G. V. Nazin, and W. Ho, *Phys. Rev. Lett.* **92**, 206102 (2004).
 - [23] A. N. Pasupathy, J. Park, C. Chang, A. V. Soldatov, S. Lebedkin, R. C. Bialczak, J. E. Grose, L. A. K. Donev, J. P. Sethna, D. C. Ralph, and P. L. McEuen, *Nano Lett.* **5**, 203 (2005).
 - [24] O. Tal, M. Krieger, B. Leerink, and J. M. van Ruitenbeek, *Phys. Rev. Lett.* **100**, 196804 (2008).
 - [25] M. Kiguchi, O. Tal, S. Wohlthat, F. Pauly, M. Krieger, D. Djukic, J. C. Cuevas, and J. M. van Ruitenbeek, *Phys. Rev. Lett.* **101**, 046801 (2008).
 - [26] H. Song, Y. Kim, Y. H. Jang, H. Jeong, M. A. Reed, and T. Lee, *Nature* **462**, 1039 (2009).
 - [27] T. Frederiksen, M. Paulsson, M. Brandbyge, and A.-P. Jauho, *Phys. Rev. B* **75**, 205413 (2007).
 - [28] D. A. Ryndyk, R. Gutiérrez, B. Song, and G. Cuniberti, in *Energy Transfer Dynamics in Biomaterial Systems*, Springer Series in Chemical Physics, Vol. 93, edited by I. Burghardt, V. May, D. A. Micha, E. R. Bittner, A. W. Castleman, J. P. Toennies, K. Yamanouchi, and W. Zinth (Springer Berlin Heidelberg, 2009) pp. 213–335.
 - [29] W. Lee, N. Jean, and S. Sanvito, *Phys. Rev. B* **79**, 085120 (2009).
 - [30] M. Knap, W. von der Linden, and E. Arrigoni, *Phys. Rev. B* **84**, 115145 (2011).
 - [31] M. Nuss, C. Heil, M. Ganahl, M. Knap, H. G. Evertz, E. Arrigoni, and W. von der Linden, *arXiv:1207.5641* (2012).
 - [32] A. J. Heeger, S. Kivelson, J. R. Schrieffer, and W. P. Su, *Rev. Mod. Phys.* **60**, 781 (1988).
 - [33] D. Sénéchal, D. Perez, and M. Pioro-Ladrière, *Phys. Rev. Lett.* **84**, 522 (2000).
 - [34] Y. Meir and N. S. Wingreen, *Phys. Rev. Lett.* **68**, 2512 (1992).
 - [35] M. Nuss, M. Knap, E. Arrigoni, and W. von der Linden, to be published.
 - [36] R. Landauer, *Philos. Mag.* **21**, 863 (1970).
 - [37] M. Büttiker, *Phys. Rev. Lett.* **57**, 1761 (1986).
 - [38] J.-X. Zhu and A. V. Balatsky, *Phys. Rev. B* **67**, 165326 (2003).
 - [39] C. Romeike, M. R. Wegewijs, W. Hofstetter, and H. Schoeller, *Phys. Rev. Lett.* **96**, 196601 (2006).

- [40] D. Rai, O. Hod, and A. Nitzan, [J. Phys. Chem. C **114**, 20583 \(2010\)](#).